Supplementary information for

Enhanced Chemiluminescence Determination of Paracetamol

Simin Emdadi,** Mohammad Hossein Sorouraddin ^b and Lynn Denanny^c

- a. Department of Analytical Chemistry, Faculty of Chemistry, University of Tabriz, Tabriz, Iran. E-mail: siminemdadi@gmail.com
- b. Department of Analytical Chemistry, Faculty of Chemistry, University of Tabriz, Tabriz, Iran. E-mail: <u>soruraddin@tabrizu.ac.ir</u>
- c. Department of Pure & Applied Chemistry, University of Strathclyde, UK. E-mail: lynn.dennany@strath.ac.uk

This file includes:

Table S1 (The concentrate rang of each parameter in 5 levels based on CCD (n=2))

Table S2 (Design matrixes generated for CCD)

Table S3 (ANOVA).

- Fig. S1 Effect of the various acids on the signal/blank ratio
- Fig. S2 Response surface plot and contour plot of CL intensity

Fig. S3 univariate optimization

Table S1 The concentrate rang of each parameter in 5 levels based on CCD (n=2)

Factor	Symbol	Level				
		α	1	0	-1	-α
H_2SO_4 (M)	X ₁	0.018	0.014	0.01	0.006	0.002
SDS % (w/v)	X ₂	6.6	5.2	3.8	2.4	1
KMnO₄(mM)	X ₃	8	6.5	5	3.5	2
Rh.6G (mM)	X_4	2.6	2	1.4	0.8	0.2

Table S2 Design matrixes generated for CCD and obtained response value (PCM 6.6 μ M).

		Coded va				
Run	X_1 (H ₂ SO ₄)	X_2 (SDS)	X ₃ (Rh.6G)	X ₄ (KMnO ₄)	Response	Predicted
1	0	0	0	0	83315	84300
2	0	0	0	0	85377	84300
3	-1	-1	-1	-1	39583	39196.2
4	0	0	2	0	36529	37458.6
5	0	2	0	0	29873	29455.3
6	0	0	0	0	82412	84300
7	1	-1	1	1	16856	15671
8	-1	1	1	1	38788	38105
9	0	-2	0	0	17092	20356.8
10	-2	0	0	0	59741	61177.3
11	-1	1	1	-1	54269	50023
12	1	1	1	1	14302	13976.2
13	-1	1	-1	1	55516	55125.5

14	0	0	0	0	85595	84300
15	-1	1	-1	-1	47875	49989.5
16	-1	-1	1	1	29541	30780.2
17	0	0	-2	0	59245	59162.5
18	1	-1	-1	1	37125	37408.3
19	0	0	0	0	84310	84300
20	1	1	-1	-1	54289	50143.2
21	1	1	1	-1	45469	46961.9
22	1	-1	-1	-1	47821	48369.5
23	2	0	0	0	46811	462218
24	-1	-1	1	-1	39654	37727.9
25	1	1	-1	1	32420	34211.7
26	0	0	0	0	35156	84300
27	-1	-1	-1	1	50930	49302.7
28	0	0	0	-2	43871	44693.1
29	0	0	0	0	84920	84300
30	0	0	0	2	21789	21814
31	1	-1	1	-1	44009	43686.5

Table S3 Analysis of Variance for Response (ANOVA)

Source	DOF	Seq SS	Adj SS	Adj MS	F-value	P-value
Regression	14	14480018288	14480018288	1034287021	508.03	0.000
Linear	4	1951443497	1951443497	487860874	239.63	0.000
H2SO4	1	335500470	335500470	335500470	164.79	0.000
SDS	1	124174053	124174053	124174053	60.99	0.000
KMnO4	1	706584572	706584572	706584572	347.07	0.000
Rh.6G	1	785184401	785184401	785184401	385.67	0.000
Square	4	11675228112	11675228112	2918807028	1433.68	0.000
H2SO4*H2SO4	1	579682710	1673544600	1673544600	822.03	0.000
SDS*SDS	1	4750360362	6304722384	6304722384	3096.81	0.000
KMnO4*KMnO4	1	1688116183	2314899007	2314899007	1137.05	0.000
Rh.6G*Rh.6G	1	4657068858	4657068858	4657068858	2287.50	0.000
Interaction	6	853346679	853346679	142224446	69.86	0.000
H2SO4*SDS	1	81355890	81355890	81355890	39.96	0.000
H2SO4*KMnO4	1	10334618	10334618	10334618	5.08	0.039
H2SO4*Rh.6G	1	443850090	443850090	443850090	218.01	0.000
SDS*KMnO4	1	2255253	2255253	2255253	1.11	0.308
SDS*Rh.6G	1	24703385	24703385	24703385	12.13	0.003
KMnO4*Rh.6G	1	290847443	290847443	290847443	142.86	0.000
Residual Error	16	32574058	32574058	2035879		
Lack-of-Fit	10	27733356	27733356	2773336	3.44	0.072
Pure Error	6	4840702	4840702	806784		
Total	30	14512592346				
R-Sq = 99.78%						
R-Sq(adj) = 99.58%						
R-Sq(pred) = 98.85%						



Fig. S1 Effect of the various acids on the signal/blank ratio. Condition: $KMnO_4$, 2.5 mM; Rh.6G, 1 mM; PCM, 6.6 μ M; SDS, 5% (w/v); acid (HCl, H₃PO4, and H₂SO₄), 0.01 M; All of the reagents dissolved in distilled water (n=5); (monitored at 560 nm).





Fig. S2 Response surface plot and contour plot of CL intensity as a function of: (A) Rh.6G and KMnO₄ concentration at H_2SO_4 , 0.01 M and SDS 3.8% (w/v); (B) Rh.6G concentration and SDS% at H_2SO_4 , 0.01 M and KMnO₄, 5 mM; (C) KMnO₄ concentration and SDS% at H_2SO_4 , 0.01 M and Rh.6G, 1.4 mM; (D) Rh.6G and H_2SO_4 concentration at KMnO₄, 5 mM and SDS, 3.8% (w/v); (E) KMnO₄ and H_2SO_4 concentration at SDS, 3.8% (w/v) and Rh.6G, 1.4 mM; (F) SDS % and H_2SO_4 concentration at KMnO₄, 5 mM and Rh.6G, 1.4 mM. All of the experiments were tested at the present of the PCM, 6.6 μ M.





Fig. S3 (A) The effect of concentration of Rh.6G. Condition: PCM, 6.6 μM; SDS, 5% (w/v); H₂SO₄ 0.05 M; KMnO₄, 2.5 Mm; (B) The effect of concentration of SDS. Condition: PCM, 6.6 μM; Rh.6G, 2 mM; H₂SO₄, 0.05 M; KMnO₄, 2.5 mM; (C) The effect of concentration of H₂SO₄. Condition: PCM, 6.6 μM; SDS, 4% (w/v); Rh.6G, 2 mM; KMnO₄, 2.5 Mm; (D) The effect of concentration of KMnO₄. Condition: PCM, 6.6 μM; SDS, 4% (w/v); Rh.6G, 2 mM; KMnO₄, 2.5 Mm; (D) The effect of concentration of KMnO₄. Condition: PCM, 6.6 μM; SDS, 4% (w/v); Rh.6G, 2 mM; KMnO₄, 2.5 Mm; (D) The effect of concentration of KMnO₄. Condition: PCM, 6.6 μM; SDS, 4% (w/v); Rh.6G, 2 mM; H₂SO₄, 0.02 M. All of the reagents dissolved in distilled water. (n=5)